Whole Core Pin-by-Pin Coupled Neutronic-Thermal-hydraulic Steady state and Transient Calculations using COBAYA3 code

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Abstract

Nowadays, coupled 3D neutron-kinetics and thermal-hydraulic core calculations are performed by applying a radial average channel approach using a meshing of one quarter of assembly in the best case. This approach does not take into account the subchannels effects due to the averaging of the physical fields and the loose of heterogeneity in the thermal-hydraulic modelization. Therefore the models do not have enough resolution to predict those subchannels effects which are important for the fuel design safety margins, because it is in the local scale, where we can search the hottest pellet or the maximum heat flux.

The UPM advanced multi-scale neutron-kinetics and thermal-hydraulics methodologies being implemented in COBAYA3 include domain decomposition by alternate core dissections for the local 3D fine-mesh scale problems (pin cells/subchannels) and an analytical nodal diffusion solver for the coarse mesh scale coupled with the thermal-hydraulic using a modelization of one channel per assembly or per quarter of assembly.

In this work, we address the domain decomposition by the alternate core dissections methodology applied to solve coupled 3D neutronic/thermal-hydraulic (N-TH) problems at the fine-mesh scale. The N-TH coupling at the cell-subchannel scale allows the treatment of the effects of the detailed TH feedbacks on cross-sections, thus resulting in better estimates of the local safety margins at the pin level.

1. INTRODUCTION

The development of nuclear technology has enabled more and more realistic vision of the phenomena that occur in a nuclear reactor, in particular in neutron and thermal-hydraulic aspects. This requires on the one hand increasing the mesh refinement of calculation used, so far involved the homogenization of large regions of the reactor core, and secondly, the resolution of the corresponding coupled equations.

To overcome those limitations, the domain decomposition methodology through alternate dissections [1] has been developed and applied to the analysis of PWR reactor cores. The work presented in this paper is focused on the implementation and validation of a neutronic/thermal-hydraulic coupling of these features, which has been performed as part of the PhD thesis of the first author. This methodology allows us to tackle the problem of calculating the full-scale core in the level of fuel rods and subchannels with a multi-scale approach. The core calculation at this level of detail allows us to consider the effects of detailed thermal-hydraulic feedback on cross sections, resulting in better estimation of local security limits in the fuel bundles.

The domain decomposition methodology was first applied in the local-global scheme used in the Spanish System of Analysis of Pressurized Water Reactors [2][3]. In the neutronic field, current to flux ratios based on the interface discontinuity factor diffusion formulation [4] are used as boundary conditions in the calculation of each subdomain problem. In the thermal-hydraulic field, cross-flows between adjacent subchannels are chosen as boundary conditions equivalents to the current to flux ratios in neutronic to connect different subdomains.

The methodology cited in the preceding paragraph has been applied to the OECD/NEA MOX Core Transient Benchmark [5], using the COBAYA3 code system [1][6] for making these multi-scale calculations. The results reported in this paper will show the goodness of this methodology to address such kind of problems.

2. DOMAIN DECOMPOSITION THROUGH ALTERNATE DISSECTIONS

The core partition in quarters of assemblies is a physically meaningful way of domain decomposition that can be applied in both neutronic and thermal-hydraulic physics [4]. Figure 1 shows a graphical representation of the level of detail considered for the fine-mesh transport corrected diffusion solver COBAYA3 and the two phase-flow code COBRA-TF [7] which provides the thermal-hydraulic subchannel solution for the cross section feedback.

The neutronic boundary conditions (BC) are the fine-mesh current to flux ratios in each cell interface, because they are independent of the level of flux in the subdomain and leave the diffusion equation in a homogeneous form. Therefore, they are insensitive to the fission source levels supposed over the core in order to converge the k-eigenvalue problem. On the other hand, the domain decomposition is unable to produce the correct source level for the core, only can improve the fission source distribution inside the subdomain. The alternate dissections scheme makes it possible to reach the true fission source distribution by “mixing” the quarters of assemblies. In that sense, the nodal solution is in charge of improving the fission source levels for the full core problem which are used to normalize the fluxes of each subdomain in the pin-by-pin solution, and hence, speeding up the overall problem convergence.

The thermal-hydraulic BC are mass injections (or sinks) at the outer open surfaces of the subdomain. Those mass injections come from the previous subchannel calculation on a different core dissection, and are derived from the cross-flows obtained in the centerplanes gaps connecting quarters of assemblies.

During the iterative solution process, the BC on the subdomain and their returned updated values on the centerplanes at the end of each computation are the information to be transmitted mainly. But also volume information is passed to initialize the values for the next subdomain computation and keep track of the convergence in the full core solution.

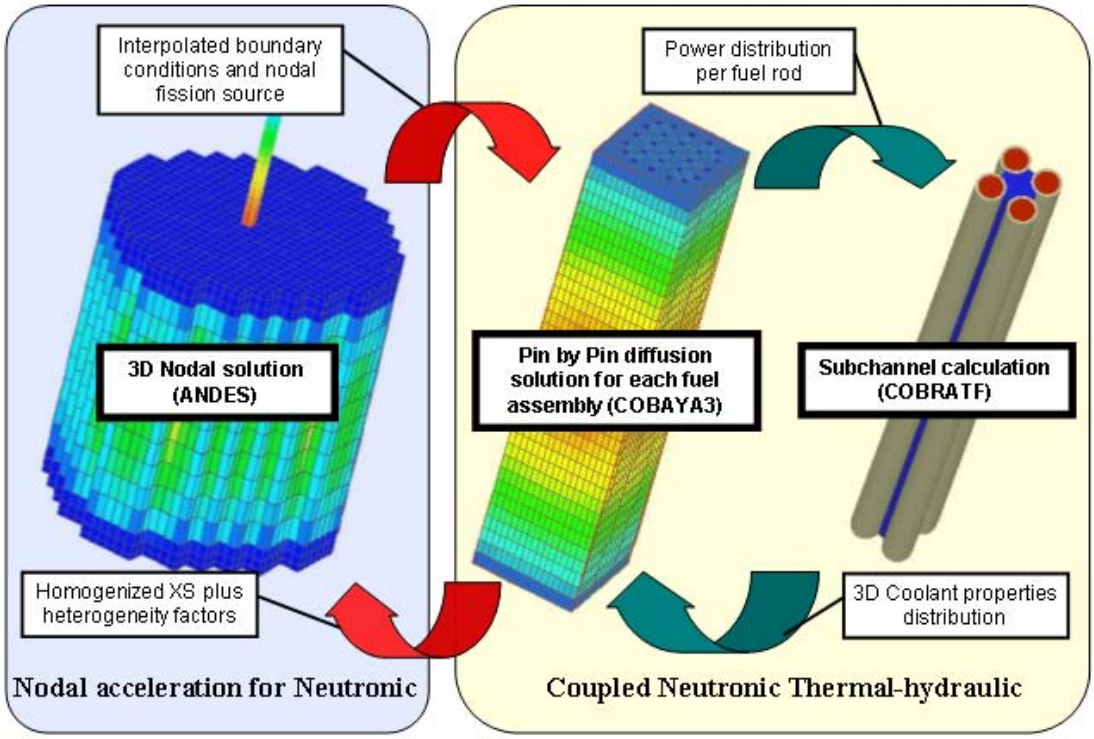

Figure 1. Overview of the multi-scale coupling scheme

To reduce computing times, each formed subdomain is solved simultaneously to other subdomains in different processors thanks to the parallelization of the solution method. The processors compute the k-eigenvalue and fission source distribution for each isolated subdomain, then new current to flux ratios are computed in the centerplanes. When convergence is reached in the full core, k-eigenvalue coincides for all the subdomains, the pin powers are stored and then used by the thermal-hydraulic code as a fixed source term.

The thermal-hydraulics solution uses a quasi-stationary method to reach the steady state conditions because, up to now, COBRA-TF does not have a steady state solution implemented. The solution initiates at zero time and a void transient is run till convergence is reached for each subdomain, then cross flows are computed in the centerplanes of the geometry which are subchannel boundaries where BC will be applied in the next dissection. Those BC are formed by the three fields exchanged between neighboring subchannels in the centerplanes of the subdomains, namely mass, enthalpy, and momentum.

After each dissection, all the subdomains are said to be in the same instant of time, and a restart case is computed for the next dissection using the updated cross flows and the already computed fields as initial conditions. Then, a comparison is established between the temperatures and densities fields computed in different iterations to decide the moment of convergence. In nominal conditions only two to three different alternate dissections are needed for the thermal-hydraulics

to converge the full core temperatures and densities distributions. Afterwards, the cell temperatures and densities are stored and used by the pin-by-pin solver to interpolate in the cross sections tables in a new pin power computation.

2.1 Convergence of the Alternate Dissections Methodology

All the development of the alternate dissections is based on the Schwarz alternating method, whose convergence is proven for overlapping subdomains [10][11]. And on the heuristic numerical performance in 2D and 2-group diffusion calculations of PWR cores [1][2].

It is possible to divide a PWR core geometry in quarters of assemblies comprehending the whole axial length, these quarters can be grouped following four alternate dissections formed by single assemblies (one color-sets), for quarters of neighboring assemblies (4 color-sets), or combinations of half assemblies in the horizontal and vertical directions (2 color-sets).

The fundamental paradigm of the alternate dissections resides in the fact that the centerplanes of each subdomain considered in this way coincides with the boundary planes of other subdomains formed in different dissections, so as to compute updated values for the fine-mesh boundary conditions in these centerplanes on each iteration. Moreover, as each of the four partitions considered fully overlap with the rest of partitions; the convergence rate of the recomputed boundary conditions is considerably faster.

Let’s suppose the fission source in each cell is fixed and also the k eigenvalue, then the boundary conditions for the next iteration can be computed from the centerplanes of each set of subdomains at the end of the current iteration; and therefore, a fully converged solution will be achieved after some iterations over the 4 dissections classes. The number of iterations at the level of the cell is very much reduced when a nodal solution using homogenized cross sections and heterogeneity factors from the pin-by-pin solution is introduced in between each set of subdomains solutions; this nodal computation is performed using the ANDES code [12] which provides an accurate solution of the fission source distribution using de ACMFD formulation [3]. The nodal values are applied to the detailed solution by interpolating the boundary conditions on each nodal face adding a piecewise constant. After the convergence of the boundary conditions, the fission source for each cell is recomputed together with the core k eigenvalue, and a new fixed source problem is solved till convergence of the full core fission source.

In this development we go one step further and the fission source problem is solved on each subdomain, getting a k eigenvalue for each one, and also solving the eigenvalue problem for the nodal acceleration. In this case, the convergence of the fission source is very much improved by the nodal solution; even more, the nodal acceleration is absolutely necessary when the problem is solved in multigroups and three dimensional geometries. The reason for that comes from the fact that the convergence of the Schwarz alternating method is not ensured for this kind of mixed eigenvalue plus boundary conditions problem.

For the case of the thermal-hydraulics, the same domain decomposition is applied; but in this case the nodal acceleration, or better the channel acceleration, is not needed because the convergence is already ensured as the source terms are not updated for each solved dissection.

The subchannel problem is found to converge in a reduced number of iterations for nominal PWR conditions, where the cross flows are not of much importance and there is no void distribution in the coolant.

In figure 2 it is shown how the errors in the currents and fission source distribution are efficiently reduced among different dissections. Those convergence rates correspond to a full length 3x3 minicore configuration with reflective boundary conditions. In this scenario, only 10 TH dissections are needed the get full convergence against 30 N ones, but the total computing time is distributed half and half between N and TH calculations. Generally, the first TH sweeps are more expensive in terms of computing time than the N because of the void transient in COBRA-TF.

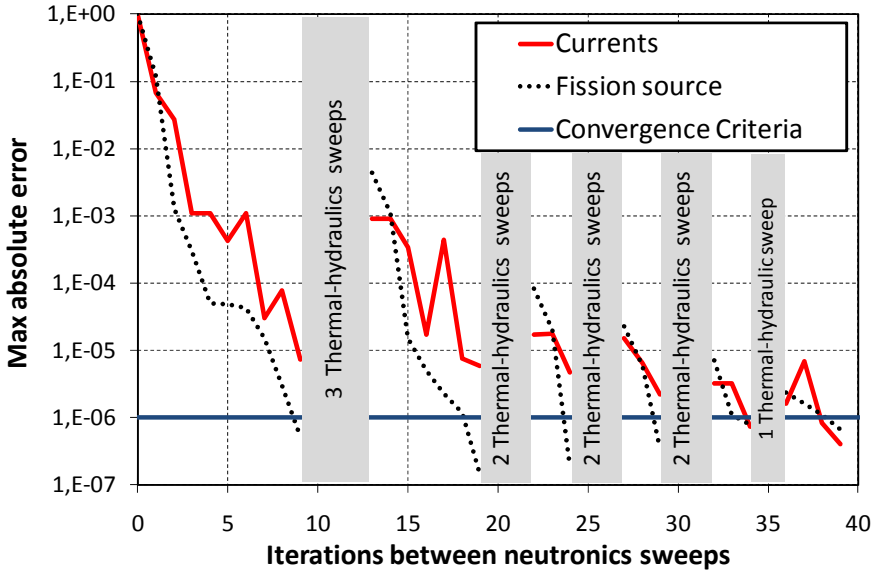

Figure 2. Convergence in a 3x3 minicore problem

3. IMPLEMENTATION IN THE COBAYA3 CODE

To reduce computing times, each formed subdomain is solved simultaneously to other subdomains in different processors. The master-slave solution method chosen uses one single reserved process to manage the information treatment; this process prepares the values to be sent to each subdomain and sends that information to one subdomain at a time. All the information is packed in a single buffer and then sent in a single hit to the MPI library, so as to avoid generating constantly all the wrap-up that accompanies message sending.

The master process sends sequentially each subdomain to free processors, meaning that they are not computing a subdomain at that time. When there are no more processors available, it waits until one finishes his computations and sends results, and then it continues sending new subdomains until the full core has been computed for the corresponding type of dissection.

Thereafter, when the fission source is being computed in a neutronic sweep, a nodal solution is performed in the master process and the interpolation values are generated. Again a new dissection, different from the previous one, begins where the updated nodal values are used to

interpolate the boundary conditions in each slave process and the nodal fission source level is used to renormalize the subdomains.

After each dissection, all the subdomains are said to be in the same instant of time, and a restart case is computed for the next dissection using the updated cross flows and the already computed fields as initial conditions. It is remarkable that the amount of information to be transmitted at the moment is 15 times more for thermal-hydraulics than for neutronics, this could be balanced with the inclusion of burnup or equilibrium Xenon in the computation for instance.

A comparison is established between the temperatures and densities fields computed at each iteration and the precedent to decide the moment of convergence. In nominal conditions only two to three different alternate dissections are needed for the thermal-hydraulics to converge the full core temperatures and densities distributions. Afterwards, the cell temperatures and densities are stored and used by the pin-by-pin solver to interpolate in the cross sections tables in a new pin power computation.

Figure 3 represents the flow chart of this coupled calculation which also applies a damping on the thermal-hydraulics solution to accelerate the convergence to the steady state and avoid oscillations. Other coupling schemes at the subdomain level are being investigated.

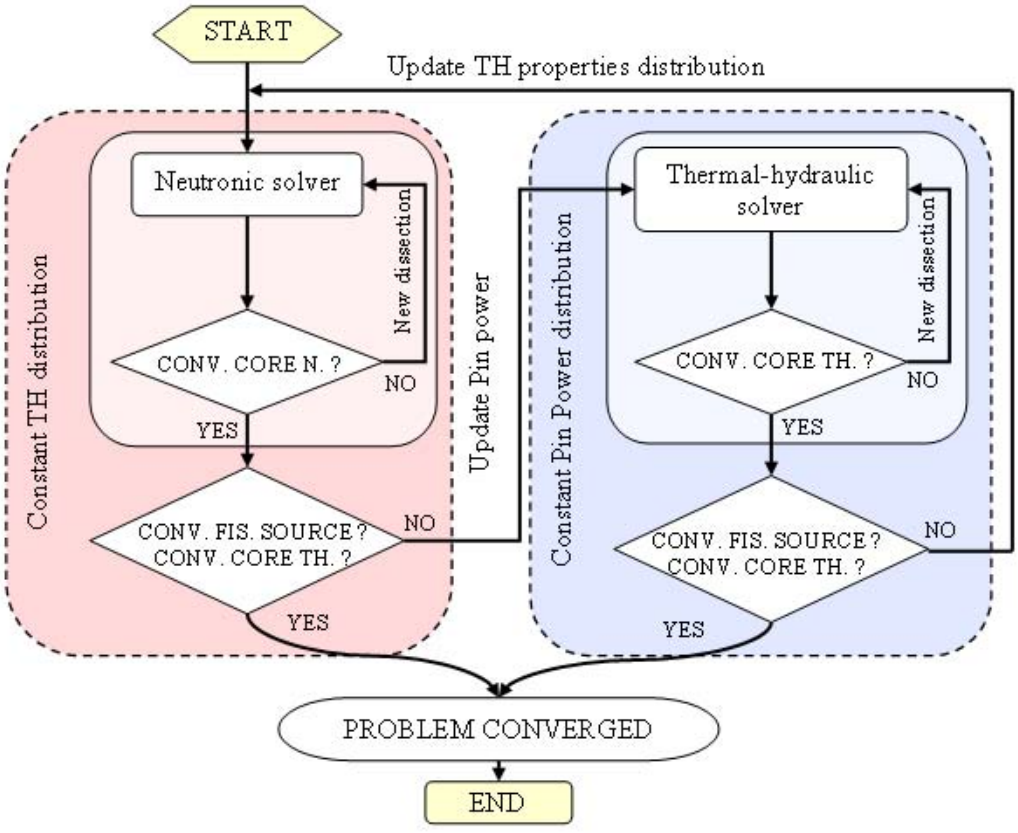

Figure 3. Implementation of the convergence logic in Alternate Dissection

After each neutronic or thermal-hydraulic full core solution, the new values are compared against the ones stored at the beginning of the alternate dissections. When the change is small enough for the pin powers and the temperatures and densities fields used in the cross-section feedback, the problem is considered solved.

3.1 Computer Requirements of the Domain Decomposition in COBAYA3

The developed code has been tested in a single 8 processors machine, a cluster of 48 processors, and a supercomputer with more than 1000 processors available. Actually, the optimum number of processors needed clearly depends on the size of the problem, thus, having more processors than the maximum number of subdomains formed, does not reduce the overall CPU time. And, on the other side, having less available processors than the maximum number of subdomains can lead to a situation in which all the subdomains are computed except one, and the execution in the master process have to wait till the last one is finished before going for a new dissection.

The master-slave solution method has been designed to tackle the memory requirements by distributing the memory containers among all the available processors. The memory required for a single fuel assembly including the whole active height is about 300 MB when using 40 axial levels in the thermal-hydraulics and 160 axial levels in the neutronics. Therefore, for a typical PWR core with 157 assemblies, the amount of memory needed is about 46 GB.

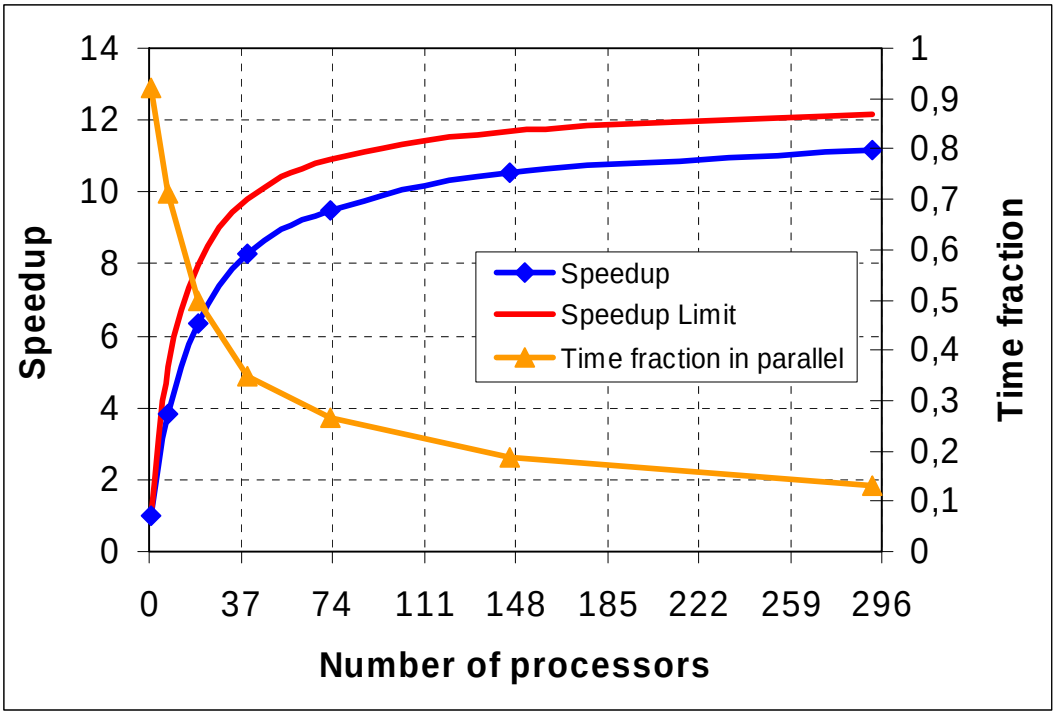

Figure 4. Speedup performance of the parallelized solution scheme

To illustrate the speedup of the parallelized neutronic solver, figure 4 shows the convergence behavior with the number of processors used to compute the ARI-1 steady-state case at HZP for PWR MOX/UO_2 benchmark in 3D with 8 energy groups. Computational times go from 4.5 hours in one processor to 0.4 hours using 128 processors.

As showed in the previous figure, the speedup saturates over 128 processors because the time fraction in the parallelized part of the code lowers its importance with increasing number of processors: the unitary benefit of adding one more processor gets lower and lower. The cause for this behavior is of course the non-parallelized part of the code which corresponds with the nodal solver and the message passing from the slaves to the subdomains.

Thus two ways of improving this performance have to be considered, one improving the nodal solver speed, may be using a lower order nodal solution and/or an also parallelized solver, and other sending less amount of memory from the master to the slaves. However, the amount of time used in the message passing time is very small when compared with the computing time, and the true gain should be in the improvement of the nodal solver performance.

4. RESULTS AND NUMERICAL VERIFICATION

The OECD/NEA/USNRC PWR MOX/UO_2 Core Transient Benchmark [5] provides homogenized pin level cross sections but without cell discontinuity factors to account for cell heterogeneities, transport and mesh size effects. It is used to compute full core results in comparison to the ones submitted in the final report. All the pin-by-pin calculations used the 8G cell cross section libraries.

First, we presented a pin-by-pin solution for the full core at HZP ARI as described in Part 3 of the benchmark specification, where each pin, cladding and surrounding coolant is homogenized in one cell. Table I shows a comparison of some parameters with DeCART transport solution which was taken as reference and the PARCS and ANDES nodal solution in 2 groups.

	DeCART	**COBAYA3**	**PARCS 2G**	**ANDES 2G**
Critical Boron	1265 ppm	1313 ppm	1341 ppm	1343 ppm
PWE (%)	ref	1.17	1.05	1.06
EWE (%)	ref	2.79	3.49	3.44

Table I. HZP 3D steady state assembly power relative error (%) with DeCART

The COBAYA3 values are found to be in between both approaches, and they would be very much improved if the interface discontinuity factors [2] would have been included in the cell library of the benchmark because of the mesh, transport and heterogeneity effects to be corrected. Table II shows the corresponding results of COBAYA3/COBRA-TF using the domain decomposition for the HFP exercise of the benchmark compared against ANDES/COBRA-TF and PARCS nodal solutions.

	COBAYA3/CTF	ANDES/CTF 8G	PARCS 8G
Critical Boron	1655.0 ppm	1672.5 ppm	1672.0 ppm
F_z	1.437	1.422	1.424
F_{xy}	1.3233	1.395	1.384
A.O.(%)	-10.25	-10.30	-9.9
$T_{Doppler}$ (ºC)	561.7	561.8	563.0
$T_{fuel\ max}$ (ºC)	1770.4	1572.8	-

Table II. MOX-part2 3D HFP steady state comparison

There is a very good agreement on the results shown in table Table II where the deviations in k_{eff} are in less than 170 pcm. Nevertheless, it can be seen how the maximum fuel temperature is almost 200ºC higher in the pin-by-pin/subchannel coupled calculation than in the nodal/channel solution. In 0 it is compared the assembly wise power distribution obtained from the pin-by-pin calculation compared with the solution provided by ANDES/CTF. The highest errors are concentrated in the periphery of the core where gradients within the assemblies are higher due to the reflector presence. Therefore, the lack of cell discontinuity factors in the cross sections library is more remarkable.

Just to give some numbers about computational times, the COBAYA3/CTF calculation took 2 days and 5 hours using 225 processors in the Magerit cluster, and the ANDES/CTF took 16 min. on a workstation. Without parallelization, the detailed calculation would take 497 days to complete on the same workstation.

	1	2	3	4	5	6	7	8
1	1,120 1,679E-02	1,390 8,561E-03	1,200 5,333E-03	1,370 7,299E-04	1,020 4,314E-03	1,110 4,955E-03	1,100 1,200E-02	0,481 1,019E-02
2	1,390 8,561E-03	1,270 8,031E-03	1,080 4,444E-03	1,200 9,167E-04	**1,300** 8,462E-04	0,974 2,669E-03	1,110 9,009E-04	0,571 1,296E-02
3	1,200 5,333E-03	1,080 4,444E-03	1,180 5,763E-03	1,330 4,060E-03	1,210 6,612E-04	1,190 3,361E-04	1,100 6,818E-03	0,474 2,152E-02
4	1,370 7,299E-04	1,200 9,167E-04	1,330 4,060E-03	1,060 6,792E-03	1,290 1,008E-03	1,180 2,627E-03	1,000 2,700E-03	0,398 7,035E-03
5	1,020 4,314E-03	**1,300** 8,462E-04	1,210 6,612E-04	1,290 1,008E-03	0,937 4,696E-03	1,120 1,339E-03	0,645 1,240E-03	
6	1,110 4,955E-03	0,974 2,669E-03	1,190 3,361E-04	1,180 2,627E-03	1,120 1,339E-03	0,843 3,084E-03	0,319 9,404E-04	
7	1,100 1,200E-02	1,110 9,009E-04	1,100 6,818E-03	1,000 2,700E-03	0,645 1,240E-03	0,319 9,404E-04		
8	0,481 1,019E-02	0,571 1,296E-02	0,474 2,152E-02	0,398 7,035E-03				

Result with CTF+DS: 0,1890

1,240E-02 Relative errors (%) with ANDES/CTF

Table III. HFP 3D steady assembly power relative error between COBAYA3/CTF and ANDES/CTF

5. CONCLUSIONS

The domain decomposition through alternate dissections has shown its potential and performance in addressing the problem of computing a full core at the scale of pin cells and subchannels. The results obtained show a good agreement compared against transport reference solutions and increase the level of confidence of the pin-by-pin fine mesh finite difference solver implementation and also of the coupled subchannel calculation with COBRA-TF.

During the implementation of the domain decomposition method, it has been clearly identify that a neutronic nodal acceleration is very convenient in order to achieve full core convergence and to speed up the solution process. For the thermal-hydraulic solution, the use of a core channel calculation does not improve the convergence in the subchannel scale and therefore it is not used.

Also coupled transient calculations at the pin cell scale have been performed with COBAYA3/COBRA-TF. However, the computing times required in these calculations are quite large because, up to now, the nodal/channel acceleration is not implemented yet in this kind of transient problems. This work is envisioned for future improvements of the method.

A pin-by-pin transport corrected diffusion computation coupled with an nine equations thermal-hydraulic model yields a level of detail useful to take as a reference calculation for comparison with coupled nodal-channel codes or to generate nodal cross sections libraries in situations where the thermal-hydraulics distribution within the fuel assemblies could be of importance in off-nominal conditions. It provides directly more accurate results on the margins at the pin-by-pin scales.

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